1,5-Dihydroxynaphthalene 83-56-7 | DTXSID2052574

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 1.59

Global applicability domain: Inside

Local applicability domain index: 5.74e-01

Confidence level: 7.58e-01

Nearest Neighbors from the Training Set

Image not found

1,5-Dihydroxynaphthalene

Measured: 1.94 Predicted: 1.59

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1,3-Naphthalenediol

Measured: 1.97 Predicted: 2.06

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1,4-Naphthalenediol

Measured: 1.90 Predicted: 1.93

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2-Acetylbenzoic acid

Measured: 0.81 Predicted: 1.33

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Benzenebutanoic acid, .gamma.-

oxo-

Measured: 1.30 Predicted: 1.43